Professor C. N. Yang and Statistical Mechanics

F. Y. Wu[1]

[1]*Department of Physics, Northeastern University, Boston, Massachusetts 02115, U.S.A.*

Abstract

Professor Chen Ning Yang has made seminal and influential contributions in many different areas in theoretical physics. This talk focuses on his contributions in statistical mechanics, a field in which Professor Yang has held a continual interest for over sixty years. His Master's thesis was on a theory of binary alloys with multi-site interactions, some 30 years before others studied the problem. Likewise, his other works opened the door and led to subsequent developments in many areas of modern day statistical mechanics and mathematical physics. He made seminal contributions in a wide array of topics, ranging from the fundamental theory of phase transitions, the Ising model, Heisenberg spin chains, lattice models, and the Yang-Baxter equation, to the emergence of Yangian in quantum groups. These topics and their ramifications will be discussed in this talk.

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I. INTRODUCTION

Statistical mechanics is the subfield of physics that deals with systems consisting of large numbers of particles. It provides a framework for relating macroscopic properties of a system, such as the occurrence of phase transitions, to microscopic properties of individual atoms and molecules.

The theory of statistical mechanics was founded by Gibbs (1834-1903) who based his considerations on earlier works of Boltzmann (1844-1906) and Maxwell (1831-1879). By the end of the 19th century, classical mechanics was fully developed and applied successfully to rigid body motions. However, after it was recognized that ordinary materials consist of 10^{23} molecules, it soon became apparent that the application of traditional classical mechanics is fruitless in explaining physical phenomena on the basis of molecular considerations. To overcome this difficulty, Gibbs proposed a statistical theory for computing bulk properties of real materials.

Statistical mechanics as proposed by Gibbs applies to all physical systems regardless of their macroscopic states. But in early years there had been doubts about whether it could fully explain physical phenomena such as phase transitions. In 1937, Mayer [1] developed the method of cluster expansions for analyzing the statistical mechanics of a many-particle system which worked well for systems in the gas phase. This offered some hope of explaining phase transitions, and the Mayer theory subsequently became the main frontier of statistical mechanical research. This was unfortunate in hindsight since, as Yang and Lee would later show (see Sec. IV), the grand partition function used in the Mayer theory cannot be continued into the condensed phase, and hence it does not settle the question it set out to answer.

This was the stage and status of statistical mechanics in the late 1930's when Professor C. N. Yang entered college.

II. A QUASI-CHEMICAL MEAN-FIELD MODEL OF PHASE TRANSITION

In 1938, Yang entered the National Southwest Associate University, a university formed jointly by National Tsing Hua University, National Peking University and Nankai University during the Japanese invasion, in Kunming, China. As an undergraduate student Yang

attended seminars given by J. S. (Zhuxi) Wang, who had recently returned from Cambridge, England, where he had studied theory of phase transitions under R. H. Fowler. These lectures brought C. N. Yang in contact with the Mayer theory and other latest developments in statistical mechanics [2–4].

After obtaining his B.S. degree in 1942, Yang continued to work on an M.S. degree in 1942-1944, and he chose to work in statistical mechanics under the direction of J. S. Wang. His Master's thesis included a study of phase transitions using a quasi-chemical method of analysis, and led to the publication of his first paper [5].

In this paper, Yang generalized the quasi-chemical theory of Fowler and Guggenheim [6] of phase transitions in a binary alloy to encompass 4-site interactions. The idea of introducing multi-site interactions to a statistical mechanical model was novel and new. In contrast, the first mentioning of a lattice model with multi-site interactions was by myself [7] and by Kadanoff and Wegner [8] in 1972 - that the 8-vertex model solved by Baxter [9] is also an Ising model with 4-site interactions. Thus, Yang's quasi-chemical analysis of a binary alloy, an Ising model in disguise, predated the important study of a similar nature by Baxter in modern-day statistical mechanics by three decades!

III. SPONTANEOUS MAGNETIZATION OF THE ISING MODEL

The two-dimensional Ising model was solved by Onsager in 1944 [10]. In a legendary footnote of a conference discussion, Onsager [11] announced without proof a formula of the spontaneous magnetization of the two-dimensional Ising model with nearest-neighbor interactions K,

$$I = \left(1 - \sinh^{-4} 2K\right)^{1/8}. \tag{1}$$

Onsager never published his derivation since, as related by him later, he had made use of some unproven results on Toeplitz determinants which he did not feel comfortable to put in print. Since the subject matter was close to his Master's thesis, Yang had studied the Onsager paper extensively and attempted to derive (1). But the Onsager paper was full of twists and turns offering very few clues to the computation of the spontaneous magnetization [12].

A simplified version of the Onsager solution by Kauffman [13] appeared in 1949. With the new insight to Onsager's solution, Yang immediately realized that the spontaneous

magnetization I can be computed as an off-diagonal matrix element of Onsager's transfer matrix. This started Yang on the most difficult and the longest calculation of his career [12].

After almost 6 months of hard work off and on, Yang eventually succeeded in deriving the expression (1) and published the details in 1952 [14]. Several times during the course of the work, the calculation stalled and Yang almost gave up, only to have it picked up again days later with the discovery of new tricks or twists [12]. It was a most formidable *tour de force* algebraic calculation in the history of statistical mechanics.

A. Universality of the critical exponent β

At Yang's suggestion, C. H. Chang [15] extended Yang's analysis of the spontaneous magnetization to the Ising model with anisotropic interactions K_1 and K_2, obtaining the expression

$$I = \left(1 - \sinh^{-2} 2K_1 \sinh^{-2} 2K_2\right)^{1/8}. \tag{2}$$

This expression exhibits the same critical exponent $\beta = 1/8$ as in the isotropic case, and marked the first ever recognition of universality of critical exponents, a fundamental principle of critical phenomena proposed by Griffiths 20 years later [16].

B. An integral equation

A key step in Yang's evaluation of the spontaneous magnetization is the solution of an integral equation (Eq. (84) in Ref. [13]) whose kernel is a product of 4 factors I, II, III, and IV. Yang pioneered the use of Fredholm integral equations in the theory of exactly solved models (see also Sec. VII A below). This particular kernel and similar ones have been used later by others, as they also occurred in various forms in studies of the susceptibility [17] and the n-spin correlation function of the Ising model [18–20].

IV. FUNDAMENTAL THEORY OF PHASE TRANSITIONS

As described in the above, the frontier of statistical mechanics in the 1930's focused on the Mayer theory and the question whether the theory was applicable to all phases of a

matter. Being thoroughly versed in the Mayer theory as well as the Ising lattice gas, Yang investigated this question in collaboration with T. D. Lee. Their investigation resulted in two fundamental papers on the theory of phase transitions [21, 22].

In the first paper [21], Yang and Lee examined the question whether the cluster expansion in the Mayer theory can apply to both the gas and condensed phases. This led them to examine the convergence of the grand partition function series in the thermodynamic limit, a question that had not previously been closely investigated. To see whether a single equation of state can describe different phases, they looked at zeroes of the grand partition function in the complex fugacity plane, again a consideration that revolutionized the study of phase transitions. Since an analytic function is defined by its zeroes, under this picture the onset of phase transitions is signified by the pinching of zeroes on the real axis. This shows that the Mayer cluster expansion, while working well in the gas phase, cannot be analytically continued, and hence does not apply, in the condensed phase. It also rules out any possibility in describing different phases of a matter by a single equation of state.

In the second paper [22], Lee and Yang applied the principles formulated in the first paper to the example of an Ising lattice gas. By using the spontaneous magnetization result (1), they deduced the exact two-phase region of the liquid-gas transition. This established without question that the Gibbs statistical mechanics holds in all phases of a matter. The analysis also led to the discovery of the remarkable Yang-Lee circle theorem, which states that zeroes of the grand partition function of a ferromagnetic Ising lattice gas always lie on a unit circle.

These two papers have profoundly influenced modern-day statistical mechanics as described in the following:

A. The existence of the thermodynamic limit

Real physical systems typically consists of $N \sim 10^{23}$ particles confined in a volume V. In applying Gibbs statistical mechanics to real systems one takes the thermodynamic (bulk) limit $N, V \to \infty$ with N/V held constant, and implicitly assumes that such a limit exists. But in their study of phase transitions [21], Yang and Lee demonstrated the necessity of a closer examination of this assumption. This insight initiated a host of rigorous studies of a similar nature.

The first comprehensive study was by Fisher [23] who, on the basis of earlier works of van Hove [24] and Groeneveld [25], established in 1964 the existence of the bulk free energy for systems with short-range interactions. For Coulomb systems with long-range interactions the situation is more subtle, and Lebowitz and Lieb established the bulk limit by making use of the Gauss law unique to Coulomb systems [26]. The existence of the bulk free energy for dipole-dipole interactions was subsequently established by Griffiths [27]. These rigorous studies led to a series of later studies on the fundamental question of the stability of matter [28].

B. The Yang-Lee circle theorem and beyond

The consideration of Yang-Lee zeroes of the Ising model opened a new window in statistical mechanics and mathematical physics. The study of Yang-Lee zero loci has been extended to Ising models of arbitrary spins [29], to vertex models [30], and to numerous other spin systems.

While the Yang-Lee circle theorem concerns zeroes of the grand partition function, in 1964 Fisher [31] proposed to consider zeroes of the partition function, and demonstrated that they also lie on circles. The Fisher argument has since been made rigorous with the density of zeroes explicitly computed by Lu and myself [32, 33]. The partition function zero consideration has also been extended to the Potts model by numerous authors [34].

The concept of considering zeroes has also proven to be useful in mathematical physics. A well-known intractable problem in combinatorics is the problem of solid partitions of an integer [35]. But a study of the zeroes of its generating function by Huang and myself [36] shows they tend toward a unit circle as the integer becomes larger. Zeroes of the Jones polynomial in knot theory have also been computed, and found to tend toward the unit circle as the number of nodes increases [37]. These findings appear to pointing to some unifying truth lurking beneath the surface of many unsolved problems in mathematics and mathematical physics.

V. THE QUANTIZATION OF MAGNETIC FLUX

During a visit to Stanford University in 1961, Yang was asked by W. M. Fairbank whether or not the quantization of magnetic flux, if found, would be a new physical principle. The question arose at a time when Fairbank and B. S. Deaver were in the middle of an experiment investigating the possibility of magnetic flux quantization in superconducting rings. Yang, in collaboration with N. Byers, began to ponder over the question [38, 39].

By the time Deaver and Fairbank [40] successfully concluded from their experiment that the magnetic flux is indeed quantized, Byers and Yang [41] have also reached the conclusion that the quantization result did not indicate a new property. Rather, it can be deduced from usual quantum statistical mechanics. This was the "first true understanding of flux quantization" [42].

VI. THE OFF-DIAGONAL LONG-RANGE ORDER

The physical phenomena of superfluidity and superconductivity have been among the least-understood macroscopic quantum phenomena occurring in nature. The practical and standard explanation has been based on bosonic considerations: the Bose condensation in superfluidity and Cooper pairs in the BCS theory of superconductivity. But there had been no understanding of a fundamental nature in substance. That was the question Yang pondered in the early 1960's [43].

In 1962, Yang published a paper [44] with the title *Concept of off-diagonal long-range order and the quantum phases of liquid helium and of superconductors*, which crystallized his thoughts on the essence of superfluidity and superconductivity. While the long-range order in the condensed phase in a real system can be understood, and computed, as the diagonal element of the two-particle density matrix, Yang proposed in this paper that the quantum phases of superfluidity and superconductivity are manifestations of a long-range order in off-diagonal elements of the density matrix. Again, this line of thinking and interpretation was totally new, and the paper has remained to be one that Yang has "always been fond of" [43].

VII. THE HEISENBERG SPIN CHAIN AND THE 6-VERTEX MODEL

After the publication of the paper on the long-range off-diagonal order, Yang experimented using the Bethe ansatz in constructing a Hamiltonian which can actually produce the off-diagonal long-range order [45]. Instead, this effort led to ground-breaking works on the Heisenberg spin chain, the 6-vertex model, and the one-dimensional delta function gas described below.

A. The Heisenberg spin chain

In a series of definitive papers in collaboration with C. P. Yang [46, 47], Yang studied the one-dimensional Heisenberg spin chain with the Hamiltonian

$$H = -\frac{1}{2}\sum\left(\sigma_x\sigma_x' + \sigma_y\sigma_y' + \Delta\sigma_z\sigma_z'\right). \tag{3}$$

Special cases of the Hamiltonian had been considered before by others. But Yang and Yang analyzed the Bethe ansatz solution of the eigenvalue equation of (3) with complete mathematical rigor, including the rigorous analysis of a Fredholm integral equation arising in the theory in the full range of Δ. The ground state energy is found to be singular at $\Delta = \pm 1$. Furthermore, this series of papers has become important as it formed the basis of ensuing studies of the 6-vertex model, the one-dimensional delta function gas and numerous other related problems.

B. The 6-vertex model

In 1967, Lieb [48] solved the residual entropy problem of square ice, a prototype of the two-dimensional 6-vertex model, using the method of Bethe ansatz. Subsequently, the solution was extended to 6-vertex models in the absence of an external field [49, 50]. These solutions share the characteristics that they are all based on Bethe ansatz analyses involving real momentum k.

In the same year 1967, Yang, Sutherland and C. P. Yang [51] published a solution of the general 6-vertex model in the presence of external fields, in which they used the Bethe ansatz with complex momentum k. But the Sutherland-Yang-Yang paper did not provide details of the solution. This led others to fill in the gap in ensuing years, often with analyses

starting from scratch, to understand the thermodynamics. Thus, the $\Delta < 1$ case was studied by Nolden [52], the $\Delta \geq 1$ case by Shore and Bukman [53, 54], and the case $|\Delta| = \infty$ by myself in collaboration with Huang *et al.* [55] The case of $|\Delta| = \infty$ is of particular interest, since it is also a 5-vertex model as well as an honeycomb lattice dimer model with a nonzero dimer-dimer interaction. It is the only known soluble interacting close-packed dimer model.

VIII. ONE-DIMENSIONAL DELTA FUNCTION GASES

A. The Bose gas

The first successful application of the Bethe ansatz to a many-body problem was the one-dimensional delta function Bose gas solved by Lieb and Liniger [56, 57]. Subsequently, by extending considerations to include all excitations, Yang and C. P. Yang deduced the thermodynamics of the Bose gas [58]. Their theoretical prediction has recently been found to agree very well with experiments on a one-dimensional Bose gas trapped on an atom chip [59].

B. The Fermi gas

The study of the delta function Fermi gas was more subtle. In a seminal work having profound and influential impacts in many-body theory, statistical mechanics and mathematical physics, Yang in 1967 produced the full solution of the delta function Fermi gas [60]. The solution was obtained as a result of the combined use of group theory and the nested Bethe ansatz, a repeated use of the Bethe ansatz devised by Yang.

One very important ramification of the Fermi gas work is the exact solution of the ground state of the one-dimensional Hubbard model obtained by Lieb and myself [61–63]. The solution of the Hubbard model is similar to that of the delta function gas except with the replacement of the momentum k by $\sin k$ in the Bethe ansatz solution. Due to its relevance in high T_c superconductivity, the Lieb-Wu solution has since led to a torrent of further works on the one-dimensional Hubbard model [64].

IX. THE YANG-BAXTER EQUATION

The two most important integrable models in statistical mechanics are the delta function Fermi gas solved by Yang [60] and the 8-vertex model solved by Baxter [9, 65]. The key to the solubility of the delta function gas is an operator relation [66] of the S-matrix,

$$Y_{jk}{}^{ab}\, Y_{ik}{}^{bc}\, Y_{ij}{}^{ab} = Y_{ij}{}^{bc}\, Y_{ik}{}^{ab}\, Y_{jk}{}^{bc}, \tag{4}$$

and for the 8-vertex model the key is a relation [67] of the 8-vertex operator,

$$U_{i+1}(u)U_i(u+v)U_{i+1}(v) = U_i(v)U_{i+1}(u+v)U_i(u). \tag{5}$$

Noting the similarity of the two relations and realizing they are fundamentally the same, in a paper on the 8-vertex model Takhtadzhan and Faddeev [68] called it the Baxter-Yang relation. Similar relations also arise in other quantum and lattice models. These relations have since been referred to as the *Yang-Baxter equation* [69, 70].

The Yang-Baxter equation is an internal consistency condition among parameters in a quantum or lattice model, and can usually be written down by considering a star-triangle relation [69, 70]. The solution of the Yang-Baxter equation, if found, often aids in solving the model itself. The Yang-Baxter equation has been shown to play a central role in connecting many subfields in mathematics, statistical mechanics and mathematical physics [71].

A. Knot invariants

One example of the role played by the Yang-Baxter equation in mathematics is the construction of knot (link) invariants. Knot invariants are algebraic quantities, often in polynomial forms, which preserve topological properties of three-dimensional knots. In the absence of definite prescriptions, very few knot invariants were known for decades. The situation changed dramatically after the discovery of the Jones polynomial by Jones in 1985 [72]. and the subsequent revelation that knot invariants can be constructed from lattice models in statistical mechanics [73].

The key to constructing knot invariant from statistical mechanics is the Yang-Baxter equation. Essentially, from each lattice model whose Yang-Baxter equation possesses a solution, one constructs a knot invariant. One example is the Jones polynomial which can be constructed from a solution of the Yang-Baxter equation of the Potts model, even though

the solution is in an unphysical regime [74]. Other examples are described in a 1992 review on knot theory and statistical mechanics by myself [75].

B. The Yangian

In 1985, Drinfeld [76] showed that there exists a Hopf algebra (quantum group) over $SL(n)$ associated with the Yang-Baxter equation (4) after the operator Y is expanded into a series. Since Yang found the first rational solution of the expanded equation, he named the Hopf algebra the *Yangian* in honor of Yang [76].

Hamiltonians with the Yangian symmetry include, among others, the one-dimensional Hubbard model, the delta function Fermi gas, the Haldane-Shastry model [77], and the Lipatov model [78]. The Yangian algebra is of increasing importance in quantum groups, and has been used very recently in a formulation of quantum entangled states [79].

X. CONCLUSION

In this talk I have summarized the contributions made by Professor Chen Ning Yang in statistical mechanics. It goes without saying that it is not possible to cover all aspects of Professor Yang's work in this field, and undoubtedly there are omissions. But it is clear from what is presented, however limited, that Professor C. N. Yang has made immense contributions to this relatively young field of theoretical physics.

A well-known treatise in statistical mechanics is the 20-volume *Phase Transitions and Critical Phenomena* published in 1972 - 2002 [80, 81]. The series covers almost every subject matter of traditional statistical mechanics. The first chapter of Volume 1 is an introductory note by Professor Yang, in which he assessed the status of the field and remarked about possible future directions of statistical mechanics.

At the conclusion he wrote:

One of the great intellectual challenges for the next few decades
is the question of brain organization.

As research in biophysics and brain memory functioning has mushroomed into a major field in recent years, this is an extraordinary prophecy and a testament to the insight and foresight of Professor Chen Ning Yang.

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